Modern Chemistry
2026, Vol. 14, No. 2, pp. 38–57
https://doi.org/10.11648/j.mc.20261402.11

Research Article

Physicochemical Investigation of Intermolecular Interactions Utilizing Ultrasonic and Viscometric Techniques in Binary Liquid Mixtures

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Abstract

Thermophysical properties of binary liquid mixtures comprising isopropyl benzene (cumene) paired with toluene, ethyl benzene, n-propyl benzene, mesitylene, tert-butyl benzene, and biphenyl were experimentally determined at 298.15 K and standard atmospheric pressure. The measured properties included density (ρ), viscosity (η), sound velocity (u), and refractive index (n), this provides valuable insight into the interactions within the mixtures and aids in predicting the behaviour of the chemical systems. In this study, the physical properties of isopropyl benzene (cumene) an important industrial chemical were measured at 298.15 K in binary mixtures with toluene, ethyl benzene, *n*-propyl benzene, mesitylene, tert-butyl benzene, and biphenyl. Using these experimental data, derived parameters including adiabatic compressibility (β_{ad}), free volume (V_f), internal pressure (p_i), surface tension (*S*), acoustic impedance (*Z*), and enthalpy (H) were evaluated as a function of composition to characterize the molecular interplay within the mixtures. The computed excess thermodynamic properties were utilized to construct novel empirical models. While these proposed models require a greater number of coefficients, they provide a substantially improved fit, yielding significantly lower standard deviations compared to traditional Redlich-Kister polynomial equations. Analysis of the mixtures revealed positive deviations for excess acoustic impedance (Z^E), excess surface tension (S^E), and excess enthalpy (H^E). The results indicated the presence of weak interactions between isopropyl benzene (cumene) and aromatic hydrocarbon molecules, Collectively, these compositional trends suggest the presence of weak to moderate intermolecular forces, driven predominantly by solute-solvent interactions and π-π stacking.

Keywords

Surface Tension, Sound Velocity, Density, Viscosity, Refractive Index, Free Volume, Enthalpy, Solute-solvent Interaction

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Received: 31 March 2026; **Accepted:** 13 April 2026; **Published:** 29 April 2026

1. Introduction

Investigating the physicochemical behavior of liquid mixtures is fundamental to understanding the nature and magnitude of intermolecular forces. While various analytical methods such as nuclear magnetic resonance, Raman and infrared spectroscopy, and dielectric measurements are routinely employed, ultrasonic techniques have emerged as highly effective, non-destructive tools for probing the structural and thermodynamic properties of liquid systems. Characterizing these systems, whether they consist of nonreactive organic molecules or complex pure compounds, is essential for establishing the relationship between a fluid's macroscopic physical properties and its internal molecular structure [1-7]. In real solutions, the mixing of dissimilar molecules frequently leads to non-ideal behavior due to synergistic structural changes and varying chemical affinities between the constituent solvents. To quantify these deviations, researchers rely on excess thermodynamic properties, which are defined as the difference between the experimentally measured values of a mixture and those predicted by ideal mixing rules [8]. These excess functions act as highly sensitive indicators of molecular association, enabling the validation of theoretical dissolution models. Furthermore, reliable thermo physical data and excess properties are indispensable for the design, optimization, and scaling of industrial chemical engineering operations, including separation, heat and mass transfer, and fluid flow processes [9-11]. The non-ideality in binary liquid mixtures is governed by a complex balance of competing intermolecular interactions. Universal dispersion forces, which are present in all mixtures, generally contribute to positive excess values. Conversely, specific interactions such as hydrogen bonding, charge-transfer complexation, and dipole-dipole or dipole-induced dipole interactions typically yield negative contributions [12]. Additionally, the dissociation of a self-associated pure component upon mixing usually leads to positive excess properties. Consequently, a transition toward increasingly negative excess values indicates robust, specific interactions between unlike molecules, resulting in closer molecular packing, decreased molar volume, and reduced compressibility. In recent years, these properties have remained subjects of active research, as they play a significant role in elucidating the behavior of complex fluid systems. Numerous researchers have made considerable efforts to evaluate internal pressure theoretically for both pure liquids and their mixtures using various thermodynamic and acoustic approaches. Fundamental thermodynamic and thermo physical properties provide essential information for understanding the non-ideal behavior of complex liquid systems, as such behavior arises from molecular interactions. The manner in which different molecules interact is important from both physical and chemical perspectives. To accurately capture these phenomena, fundamental physical properties such as density, viscosity, refractive index, and ultrasonic velocity must be measured. These baseline metrics allow for the evaluation of critical derived thermodynamic parameters, including internal pressure, free volume, and isentropic compressibility. These specific parameters have attracted considerable interest among chemists and engineers because they provide profound insights into localized liquid structure, molecular clustering, and dipolar interactions. To further explore these interaction dynamics, the present study investigates binary liquid mixtures of isopropyl benzene (cumene) paired with selected aromatic hydrocarbons across the entire composition range at a constant temperature of 298.15 K. By experimentally determining the density (ρ), viscosity (η), sound velocity (u), and refractive index (n), we calculate key derived parameters: adiabatic compressibility, surface tension (S), acoustic impedance (Z), free volume (Vf), internal pressure (pi), and enthalpy (H). The evaluation of these parameters, alongside their corresponding excess functions, provides a comprehensive quantitative framework to assess the specific type and extent of solute-solvent interactions occurring within these aromatic systems.

2. Experimental Procedure

2.1. Chemical

The chemical reagents utilized in this investigation are detailed in Table 1, which outlines their respective suppliers, CAS registry numbers, and mass fraction purities. Because the procured chemicals possessed high initial purity (≥99.0%), they were deemed highly suitable for the experiments. To confirm the reliability of these reagents prior to mixture preparation, baseline physical properties specifically density (ρ), viscosity (η), ultrasonic velocity (u), and refractive index (n) were experimentally evaluated. The reliability of the experimental density (ρ) [15, 18, 19, 23, 24, 28], viscosity (η) [21, 22, 28, 30], ultrasonic velocity (u) [19, 20, 23, 25, 33, 34], and refractive index (n) [23-25, 38-40] was assessed by comparing the experimental data of pure components with the corresponding literature values at studied temperature 298.15 K are reported in Table 2 and the agreement between the values obtained in the present study and the literature was found good.

Table 1. *Details of the chemicals used, including their CAS Registry Numbers and mass fraction purities, are provided in Table 1.*

Component	Formula	CAS Reg. No.	Supplier	Mass Fraction Purity (%)	Water-Content	Method Purity analysis method
Cumene	C_9H_{12}	80-15-9	CDH,(P)Ltd. New Delhi, India	99.0%	0.1%	Double distillation

Component	Formula	CAS Reg. No.	Supplier	Mass Fraction Purity (%)	Water-Content	Method Purity analysis method
Mesitylene	C9H12	108-67-8	CDH,(P)Ltd. New Delhi, India	99.0%	0.01%	Double distillation
Ethyl benzene	C8H10	100-41-4	CDH,(P)Ltd. New Delhi, India	99.0%	0.1%	Double distillation
Toluene	C7H8	108-88-3	CDH,(P)Ltd. New Delhi, India	99.0%	0.1%	Double distillation
n-Propyl benzene	C9H12	103-65-1	CDH,(P)Ltd. New Delhi, India	99.0%	0.01%	Double distillation
t-Butyl benzene	C10H14	98-06-6	CDH,(P) Ltd. New Delhi, India	99.0%	0.1%	Double distillation
Biphenyl	C12H10	92-52-4	CDH,(P) Ltd. New Delhi, India	99.0%	0.05%	Double distillation

2.2. Measurements

This study evaluated six distinct binary liquid systems consisting of isopropyl benzene (cumene) paired with ethyl benzene, toluene, mesitylene, n-propyl benzene, tert-butyl benzene, and biphenyl. Before preparing the mixtures, the reagents were subjected to standard drying and distillation protocols as detailed by Zhao et al. [13] and standard literature [14]. For instance, cumene was dried over anhydrous K_2CO_3, filtered, and fractionally distilled, with the initial and final fractions discarded. The processed liquids were subsequently stored over freshly activated molecular sieves in opaque glass containers to prevent ambient moisture absorption. All binary mixtures were prepared gravimetrically across the complete mole fraction spectrum. To completely eliminate evaporation during transfer, the exact required masses of each component were injected into specialized, sealed glass-stoppered vials using airtight syringes. Mass determinations were conducted using a high-precision electronic analytical balance (Citizen Scale Pvt. Ltd., Mumbai, India) with a readability of ±0.1 mg, yielding a maximum mole fraction uncertainty of ±0.0005. To guarantee compositional stability and prevent environmental degradation, fresh solutions were formulated for each system immediately prior to analysis, with all thermo physical and acoustic assessments executed on the exact same day of preparation.

2.2.1. Density

Density evaluations for both the pure components and their corresponding binary mixtures were conducted using a custom borosilicate glass relative density (R.D.) bottle equipped with a 25 cm^3 bulb. Prior to sample analysis, the apparatus was rigorously calibrated at 298.15 K utilizing triple-distilled and conductivity water (specific conductance less than $1 \times 10^6\ \Omega^{-1}$). During data collection, the completely sealed, bubble-free R.D. bottle was submerged in a precision thermostated water bath (MSI Goyal Scientific, Meerut, India) to guarantee absolute thermal equilibrium. The maximum estimated uncertainty for the recorded density values was $\pm 0.5\ kg \cdot m^{-3}$.

2.2.2. Sound Velocity

Acoustic properties were evaluated using a 10 mL multi-frequency ultrasonic interferometer (Model F80D, Mittal Enterprises, India). This apparatus features a 3 MHz high-precision frequency generator paired with a double-walled brass measuring cell. Following initial calibration with standardized water and benzene, the instrument determined the ultrasonic velocity by precisely measuring the wavelength generated by the internal quartz crystal. Thermal stability was maintained throughout the experiment by circulating water from a thermostated bath through the cell jacket. The standard equation:

$$U = \lambda . F \tag{1}$$

was utilized to compute the final ultrasonic velocity (U), where λ is the acoustic wavelength and *f*is the applied frequency. The standard uncertainty for these measurements was evaluated to be $0.1 m \cdot s^{-1}$.

2.2.3. Viscosity

An essential tool for examining at varying temperature, the way molecules interact with each other is a fundamental part of how they behave in binary liquid mixtures is viscosity (η). Process design in the petroleum, petrochemical etc. that involve this transport property is important in processes such as fluid transport, mixing and agitation, heat transfer, and concentration operations. Compared to pure substances, estimating the viscosity of a mixture is more difficult. It is additionally employed to determine the fluid's viscosity index, which aids in the liquid's designation. By separating surfaces, the proper viscosity of lubrication oil protects against wear and tear and lowers friction. By understanding viscosity, one can determine the engine oil's lifespan and optimal performance. Pharmaceutical companies provide medications to coat the throat, such as cough syrup, which has a high viscosity yet is still drinkable. Because of its high viscosity, gum is employed to hold the mating part firmly until its adhering action is finished.The kinematic viscosity (η) of the experimental fluids was ascertained via a suspended-level Ostwald viscometer, characterized by a 15 mL reservoir, a 90 mm capillary length, and a 0.5 mm internal diameter. Following rigorous calibration at 298.15 K utilizing triple-distilled water, benzene, and methanol, sample efflux times were recorded using an electronic chronometer with a of ±0.015 resolution. To guarantee mathematical accuracy, a minimum of four reproducible flow-time readings were averaged for each composition, while a glass seal was utilized to prevent evaporative losses during the runs. Viscosity was subsequently calculated using the established standard relation:

$$\frac{\eta}{\rho} = at - \frac{b}{t} \qquad (2)$$

Where *t* represents the efflux time, and a and b denote the characteristic viscometric constants. The calculated uncertainty for the dynamic viscosity was determined to be ±0.008 mPa.s.

2.2.4. Refractive Index

Optical refractive indices were measured using an Abbe refractometer (Model R-8, Mittal Enterprise, New Delhi) connected to a digital thermo stated water circulation bath to ensure strictly isothermal conditions at 298.15 K. Calibration was verified prior to measurement using distilled water, n-hexane, and benzene. For the sample analysis, a standard test piece was aligned using a drop of mono bromo naphthalene. The refractive index was determined by precisely aligning the light-dark demarcation line with the instrument's optical crosshairs. At 298.15 K, the refractive indices of the pure liquids namely isopropyl benzene (cumene), ethyl benzene, mesitylene, *n*-propyl benzene, *tert*-butyl benzene, and biphenyl were measured as 1.4889, 1.4935, 1.4967, 1.4856, 1.4909, and 1.4754, respectively. These values are in good agreement with those reported in the literature, thereby confirming the reliability of the experimental procedure. The uncertainty associated with the refractive index measurements was estimated to be within ±0.06%.

Table 2. *Viscosity (η), sound velocity (u), and density (ρ) values for pure components at 298.15K and atmospheric pressure are compared between experimental andliterature values.*

Compound	**ρ(g.cm^{-3})**		**u(m.s^{-1})**		**η (mPas)**		**Refractive index(n)**	
	Observed	**Literature**	**Observed**	**Literature**	**Observed**	**Literature**	**Observed**	**Literature**
Cumene	0.8532	0.8581[26]	1326	1325[31]	0.7337	0.7337[26]	1.4889	1.4889[24]
		0.5574[27]		1308[35]		0.7390[27]		1.4886[25]
Mesitylene	0.8616	0.8612[23]	1338	1336[23]	0.6449	0.6486[32]	1.4967	1.4967[25]
		0.8611[24]		1336[25]		0.6600[37]		1.4968[24]
Ethyl benzene	0.8674	0.8620[16]	1324	1312[16]	0.6345	0.6280[16]	1.4566	1.4932[38]
		0.8626[17]		1318[36]		0.6373[16]		1.4931[23]
Toluene	0.8576	0.8624[15]	1306	1307[19]	0.5527	0.5525[21]	1.4841	1.4940[23]
		0.8622[18]		1309[20]		0.5531[22]		1.4981[38]
n-Propyl benzene	0.8624	0.8577[28]	1315	1320[33]	0.7931	0.7995[30]	1.4856	1.4896[39]
		0.8577[29]		1320[34]		0.7827[28]		1.4889[40]
t-butyl benzene	0.8624	0.8624[24]	1316	1315[23]	0.7449	NA	1.4909	1.4901[24]
		0.8622[23]		1315[25]		NA		1.4902[25]
Biphenyl	0.7920	NA	1118	NA	0.6108	NA	1.4754	NA

NA: Data not available.

2.3. Modeling

Redlich-Kister Equation

To mathematically correlate the derived excess thermodynamic properties of the binary systems, the well-established Redlich-Kister (RK) polynomial model was employed [41]. This empirical expression is widely utilized to represent any given excess property (denoted as Y^E) as a function of the respective mole fractions of the constituent liquids. The general formofthe Redlich-Kister equation is expressed as:

$$Y = x_1 x_2 \sum_{j=1}^{P} A_{j-1}(x_1 - x_2)^{j-1} \quad (3)$$

In this mathematical relationship, Y^E represents the specific excess parameter being analyzed (such as excess adiabatic compressibility, excess surface tension, excess acoustic impedance, excess refractive index, excess free volume, excess internal pressure, or excess enthalpy). The terms x_1 and x_2 correspond to the mole fractions of the primary solvent (isopropyl benzene) and the secondary aromatic hydrocarbon, respectively.

The adjustable polynomial coefficients are represented by $aj-1$ which are determined via a least-squares regression analysis, while the summation occurs over the polynomial degree p. To thoroughly evaluate the validity and accuracy of this empirical fit, standard statistical metrics most notably the standard deviation were calculated to quantify the precision and consistency between the experimental observations and the model's predicted values.

3. Results and Discussion

The experimentally measured baseline thermo physicalproperties namely density (ρ), ultrasonic velocity (u), viscosity (η), and refractive index (n) for the binary mixtures of isopropyl benzene (cumene) paired with ethyl benzene, toluene, mesitylene, n-propyl benzene, tert-butyl benzene, and biphenyl at a constant temperature of 298.15 K are systematically documented in Table 3.

Table 3. *Binary mixtures of isopropyl benzene and aromatic hydrocarbons at 298.15K were measured for refractive index (n), density (ρ), sound velocity (u), and viscosity (η).*

Mole fraction-Cumene (x_1)	**Density (ρ)g.cm^{-3}**	**Viscosity (η)mPa.s**	**Speed ofSound (u)ms^{-1}**	**Refractive index (n)**	**Adiabatic compressibility(β_{ad}) ×10^{-7}Pa^{-1}**	**Free Volume V_f × 10^{-7} M^3 mol^{-1}**	**Internal pressure p_i × 10^5 / Nm^{-2}**	**Enthalpy (H) ×10^{-6} (J.mol^{-1})**	**Surface tension (S) ×10^{-3}/ N.m^{-1}**	**Acoustic impedance (Z) ×10^{-2}g.cm.s^{-1}**
Isopropyl benzene + ethyl benzene										
0.0000	0.8630	0.6345	1308	1.4935	0.6773	0.3512	2.8014	3.4463	0.26128	11.2880
0.1193	0.8612	0.6472	1310	1.4925	0.6763	0.3526	2.7754	3.4737	0.26165	11.3042
0.2209	0.8600	0.6633	1314	1.4915	0.6758	0.3537	2.7541	3.4973	0.26221	11.3109
0.3312	0.8596	0.6715	1316	1.4910	0.6751	0.3549	2.7294	3.5202	0.26264	11.3123
0.4397	0.8592	0.3882	1317	1.4905	0.6745	0.3561	2.7064	3.5438	0.26297	11.3243
0.5319	0.8588	0.6931	1318	1.4901	0.6739	0.3571	2.6853	3.5610	0.26317	11.3276
0.6395	0.858	0.7042	1320	1.4895	0.6721	0.3582	2.6608	3.5794	0.26328	11.3315
0.7301	0.8572	0.7124	1321	1.4894	0.6709	0.3591	2.6378	3.5908	0.26331	11.3328
0.8315	0.8564	0.7198	1322	1.4892	0.6694	0.3601	2.6119	3.6018	0.26343	11.3334
0.9313	0.8554	0.7249	1324	1.4890	0.6681	0.3611	2.5875	3.6137	0.26355	11.3288
1.0000	0.8532	0.7337	1326	1.4889	0.6666	0.3616	2.5691	3.6191	0.26366	11.3134
Isopropyl benzene + toluene										
0.0000	0.8672	0.5527	1312	1.4963	0.6699	0.3462	3.1354	3.3313	0.26375	11.3777
0.1193	0.8628	0.5801	1314	1.4955	0.6697	0.3481	3.0683	3.3875	0.26375	11.3749
0.2209	0.8612	0.6046	1315	1.4950	0.6695	0.3498	3.0110	3.4302	0.26374	11.3702
0.3312	0.8600	0.6293	1316	1.4946	0.6693	0.3516	2.9488	3.4725	0.26374	113657
0.4397	0.8592	0.6457	1318	1.4940	0.6691	0.3534	2.8878	3.5100	0.26374	11.3671
0.5319	0.8584	0.6706	1319	1.4938	0.6690	0.3548	2.8356	3.5375	0.26373	11.3573
0.6395	0.8576	0.6869	1320	1.4928	0.6686	0.3564	2.7745	3.5643	0.26371	11.3447
0.7301	0.8568	0.7032	1321	1.4918	0.6682	0.3577	2.7228	3.5824	0.26371	11.3355
0.8315	0.8556	0.7191	1322	1.4900	0.6677	0.3592	2.6652	3.5998	0.26368	11.3281
0.9313	0.8544	0.7266	1324	1.4898	0.6671	0.3606	2.6085	3.6130	0.26368	11.3208

Mole fraction-Cumene (x_1)	**Density (ρ)$g.cm^{-3}$**	**Viscosity (η)mPa.s**	**Speed ofSound (u)ms^{-1}**	**Refractive index (n)**	**Adiabatic compressibility(β_{ad})$\times10^{-7}Pa^{-1}$**	**Free Volume $V_f \times 10^{-7} M^3 mol^{-1}$**	**Internal pressure $p_i \times 10^5$ / Nm^{-2}**	**Enthalpy (H)$\times10^{-6}$ ($J.mol^{-1}$)**	**Surface tension (S)$\times10^{-3}$/ $N.m^{-1}$**	**Acoustic impedance (Z) $\times10^{-2}g.cm.s^{-1}$**
1.0000	0.8532	0.7337	1326	1.4889	0.6666	0.3616	2.5691	3.6191	0.26366	11.3134
Isopropyl benzene + meistylene										
0.0000	0.8616	0.6449	1338	1.4967	0.6483	0.4753	2.3605	3.2715	0.26205	11.5282
0.1193	0.8612	0.6216	1336	1.496	0.6509	0.4698	2.3875	3.3161	0.26224	11.5116
0.2209	0.8608	0.6384	1335	1.4955	0.6530	0.4618	2.4092	3.3527	0.26242	11.4976
0.3312	0.8604	0.6551	1334	1.4950	0.6552	0.4546	2.4324	3.3913	0.26260	114823
0.4397	0.86	0.6718	1333	1.4945	0.6574	0.4486	2.4556	3.4302	0.26278	11.4724
0.5319	0.8596	0.6885	1332	1.1494	0.6591	0.4356	2.4756	3.4633	0.26294	11.4558
0.6395	0.8592	0.6967	1331	1.4930	0.6608	0.4216	2.4975	3.4999	0.26311	11.4445
0.7301	0.8588	0.7048	1330	1.4920	0.6626	0.4085	2.5158	3.5304	0.26325	11.4141
0.8315	0.8584	0.7130	1329	1.4910	0.6643	0.3942	2.5364	3.5647	0.26340	11.3703
0.9313	0.8576	0.7293	1328	1.4900	0.6658	0.3751	2.5568	3.5985	0.26355	11.3485
1.0000	0.8532	0.7337	1326	1.4889	0.6666	0.3616	2.5691	3.6191	0.26366	11.3134
Isopropyl benzene + n-propyl benzene										
0.0000	0.8624	0.7931	1315	1.4856	0.6706	0.3167	2.7143	3.7622	0.26375	11.3406
0.1193	0.8620	0.7896	1316	1.4859	0.6703	0.3236	2.6986	3.7483	0.26374	11.3439
0.2209	0.8618	0.7884	1317	1.4862	0.6700	0.3298	2.6846	3.7363	0.26373	11.3499
0.3312	0.8614	0.7724	1318	1.4865	0.6669	0.3361	2.6698	3.7230	0.26372	11.3592
0.4397	0.8604	0.7664	1319	1.4868	0.6694	0.3417	2.6550	3.7090	0.26371	11.3573
0.5319	0.8596	0.7626	1320	1.4870	0.6692	0.3462	2.6421	3.6976	0.26371	11.3553
0.6395	0.8588	0.7558	1321	1.4872	0.6686	0.3508	2.6258	3.6788	0.26370	11.3480
0.7301	0.8584	0.7524	1322	1.4875	0.6681	0.3544	2.6111	3.6634	0.26369	11.3434
0.8315	0.8576	0.74630	1324	1.4880	0.6676	0.3578	2.5956	3.6474	0.26368	11.3361
0.9313	0.8560	0.7422	1325	1.4885	0.6669	0.3602	2.5808	3.6323	0.26367	11.3314
1.0000	0.8532	0.7337	1326	1.4889	0.6666	0.3616	2.5691	3.6191	0.26366	11.3134
Isopropyl benzene + t-butyl benzene										
0.0000	0.8624	0.7449	1316	1.4909	0.6695	0.4105	2.3043	3.5665	0.26229	11.3492
0.1193	0.8620	0.7445	1317	1.4908	0.6699	0.4055	2.3372	3.5798	0.26245	11.3525
0.2209	0.8612	0.7440	1318	1.4907	0.6690	0.4012	2.3648	3.5895	0.26260	11.3506
0.3312	0.8604	0.7436	1319	1.4906	0.6691	0.3978	2.3948	3.5986	0.26275	11.3487
0.4397	0.8596	0.7420	1320	1.4905	0.6689	0.3946	2.4242	3.6066	0.26290	11.3467
0.5319	0.8586	0.7398	1321	1.4904	0.6684	0.3906	2.4488	3.6136	0.26302	11.3421
0.6395	0.8572	0.7389	1322	1.4900	0.6680	0.3846	2.4768	3.6164	0.26318	11.3401
0.7301	0.8564	0.7373	1323	1.4899	0.6677	0.3788	2.5003	3.6185	0.26330	11.3355
0.8315	0.8556	0.7364	1324	1.4898	0.6673	0.3722	2.5266	3.6206	0.26344	11.3281
0.9313	0.8548	0.7351	1325	1.4896	0.6669	0.3656	2.5521	3.6215	0.26357	11.3208
1.0000	0.8532	0.7337	1326	1.4889	0.6666	0.3616	2.5691	3.6191	0.26366	11.3134

Mole fraction-Cumene (x_1)	Density (ρ)g.cm^{-3}	Viscosity (η)mPa.s	Speed ofSound (u)ms^{-1}	Refractive index (n)	Adiabatic compressibility(β_{ad})×10^{-7}Pa^{-1}	Free Volume V_f × 10^{-7} M^3 mol^{-1}	Internal pressure p_i × 10^5 / Nm^{-2}	Enthalpy (H)×10^{-6} (J.mol^{-1})	Surface tension (S)×10^{-3}/ N.m^{-1}	Acoustic impedance (Z) ×10^{-2}g.cm.s^{-1}
Isopropyl benzene + biphenyl										
0.0000	0.7920	0.6108	1118	1.4754	0.9989	0.6809	1.6766	2.9829	0.24088	8.8546
0.1193	0.7956	0.6215	1144	1.4750	0.9694	0.6498	1.7844	3.0951	0.24360	9.1519
0.2209	0.8036	0.6357	1174	1.4765	0.9347	0.6314	1.8761	3.1839	0.24593	9.4047
0.3312	0.8084	0.6510	1186	1.4796	0.8970	0.6124	1.9754	3.2722	0.24846	9.6852
0.4397	0.8144	0.6710	1198	1.4805	0.8600	0.5875	2.0732	3.3516	0.25093	9.9528
0.5319	0.8248	0.6932	1212	1.4815	0.8281	0.5576	2.1553	3.4120	0.25303	10.1780
0.6395	0.8276	0.7308	1242	1.4828	0.7910	0.5202	2.2509	3.4725	0.25548	10.4378
0.7301	0.8324	0.7161	1274	1.4845	0.7597	0.4827	2.3315	3.5183	0.25753	10.6598
0.8315	0.8436	0.7215	1286	1.4865	0.7248	0.4428	2.4210	3.5623	0.25983	10.9071
0.9313	0.8484	0.7295	1300	1.4875	0.6904	0.4006	2.5095	3.5997	0.26210	11.1494
1.0000	0.8532	0.7337	1326	1.4889	0.6666	0.3616	2.5691	3.6191	0.26366	11.3134

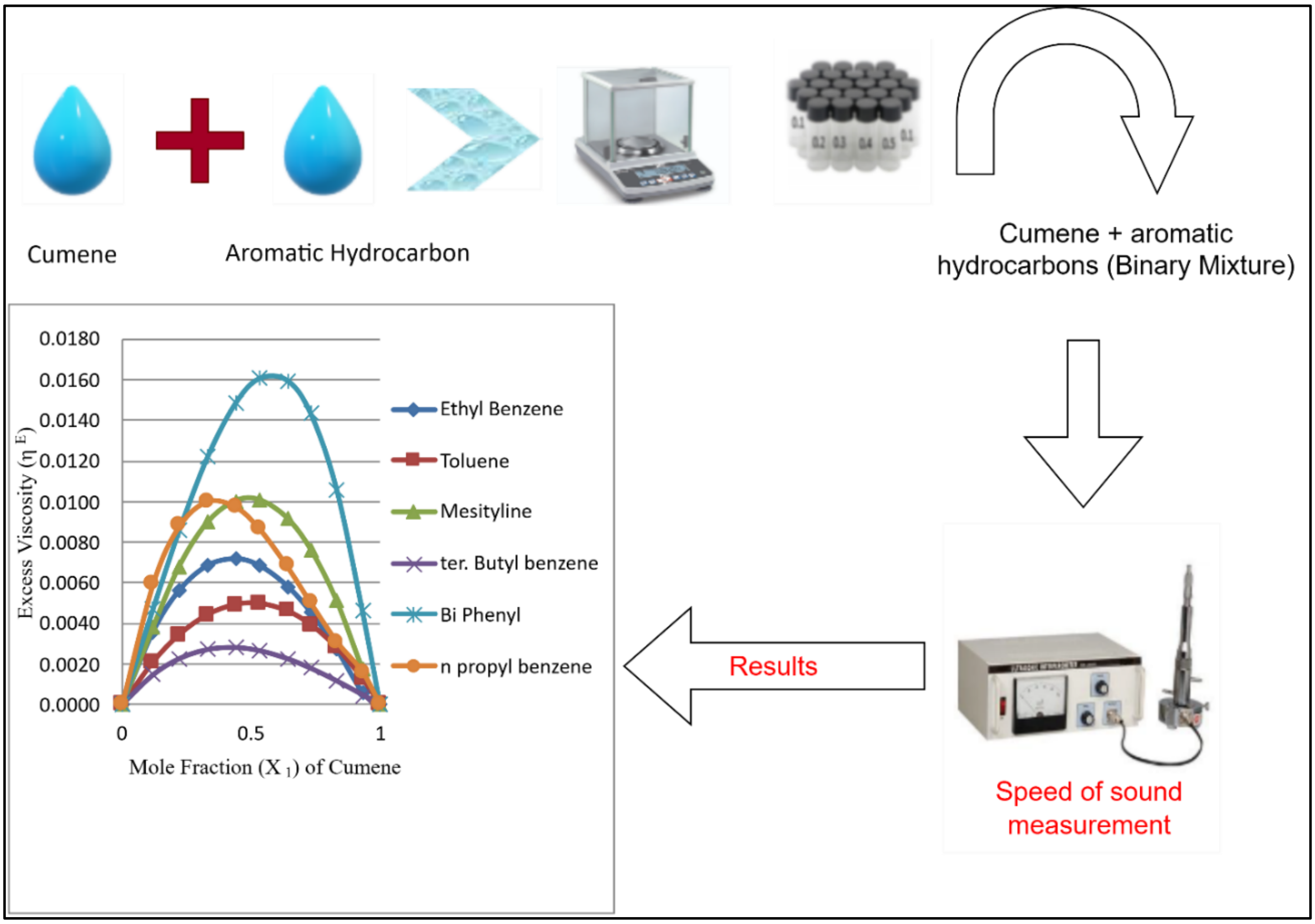

Figure 1. *Molecular interactions between aromatic hydrocarbons and isopropyl benzene (cumene) at 298.15K.*

Utilizing these fundamental measurements, a series of critical derived thermodynamic and acoustic parameters were evaluated to further characterize the fluid systems. These parameters, which include adiabatic compressibility (β_{ad}), free volume (V_f), internal pressure (p_i), enthalpy (H), acoustic impedance (Z), and surface tension (S), are also presented in Table 3. To quantify the non-ideal behavior of these mixtures, the corresponding excess thermodynamic functions were calculated and are summarized in Table 4.

Table 4. Thermodynamic parameters over flowing(β_{ad}^E, n^E, V_f^E, p_i^E, H^E, S^E, and Z^E) for a binary combination consisting of isopropyl benzene (1) + aromatic hydrocarbons (2) at 298.15.

Mole fraction 1,3-Dioxolane (x_1)	Excess adiabatic compressibility $\beta_{ad}^E \times 10^{-7}$/ Pa^{-1}	Excess refractive index (n^E) $\times 10^4$	Excess Free Volume $V_f^E \times 10^{-7}$ M^3mol^{-1}	Excessinternal pressure $p_i^E \times 10^5$/ N m^{-2}	Excess Enthalpy $H^E \times 10^{-4}$ (J.mol^{-1})	Excess Surface tension (S^E) $\times 10^5$ / N.m^{-1}	Excess Acoustic impedance (Z^E) $\times 10^{-2}$g.cm.s^{-1}
isopropyl benzene + ethyl benzene							
0.0000	0.0000	0.00	0.0000	0.0000	0.0000	0.0000	0.0000
0.1193	0.0006	1.6	0.0123	21.1098	0.6857	0.2379	0.8754
0.2209	0.0010	2.2	0.0206	39.5149	1.2822	0.4209	1.4266
0.3312	0.0014	2.7	0.0281	56.1230	1.6668	0.5309	2.0071
0.4397	0.0017	3.0	0.0333	67.6464	2.1499	0.5605	2.4819
0.5319	0.0018	3.0	0.0356	72.6363	2.2788	0.5330	2.7511
0.6395	0.0018	2.8	0.0351	71.6712	2.2607	0.4496	2.8413
0.7301	0.0016	2.5	0.0316	64.2368	1.8323	0.3445	2.6765
0.8315	0.0012	1.9	0.0238	47.6727	1.1871	0.1976	2.1711
0.9313	0.0005	1.1	0.0117	21.7987	0.6445	0.0318	1.2824
1.0000	0.0000	0.00	0.0000	0.0000	0.0000	0.0000	0.0000
isopropyl benzene + toluene							
0.0000	0.0000	0.00	0.0000	0.0000	0.0000	0.0000	0.0000
0.1193	0.0016	4.1	0.0119	4.8505	2.1838	0.0828	0.5663
0.2209	0.0033	6.4	0.0226	8.2950	3.5351	0.1441	0.9464
0.3312	0.0052	7.8	0.0311	10.9872	4.5909	0.1942	1.1641
0.4397	0.0067	7.9	0.0360	12.5109	5.2191	0.2246	1.2107
0.5319	0.0077	7.1	0.0373	12.8830	5.3108	0.2339	1.1429
0.6395	0.0080	5.1	0.0351	12.1922	4.8930	0.2237	0.9657
0.7301	0.0075	3.6	0.0302	10.6290	4.0998	0.1958	0.7553
0.8315	0.0058	1.3	0.0210	7.7685	2.9161	0.1420	0.4772
0.9313	0.0028	0.1	0.0080	3.7605	1.3671	0.0641	0.1829
1.0000	0.0000	0.00	0.0000	0.0000	0.0000	0.0000	0.0000
isopropyl benzene + meistylene							
0.0000	0.0000	0.00	0.0000	0.0000	0.0000	0.0000	0.0000
0.1193	0.0040	2.6	0.0078	16.0060	0.3054	0.0661	0.8414
0.2209	0.0066	5.0	0.0133	25.0779	0.4347	0.1385	1.7902
0.3312	0.0087	7.4	0.0177	32.3845	0.4615	0.2084	2.8454

Mole fraction 1,3-Dioxolane (x_1)	**Excess adiabatic compressibility $\beta_{ad}^E \times 10^{-7}$/ Pa^{-1}**	**Excess refractive index (n^E) × 10^4**	**Excess Free Volume $V_f^E \times 10^{-7}$ M^{3}mol^{-1}**	**Excessinternal pressure p_i^E × 10^5/ N m^{-2}**	**Excess Enthalpy H^E × 10^{-4} (J.mol^{-1})**	**Excess Surface tension (S^E) × 10^5 / N.m^{-1}**	**Excess Acoustic impedance (Z^E) × 10^{-2}g.cm.s^{-1}**
0.4397	0.0099	9.3	0.0202	36.7306	0.5849	0.2608	3.7452
0.5319	0.0103	10.3	0.0209	38.0133	0.6884	0.2867	4.2780
0.6395	0.0098	10.5	0.0199	36.4840	0.6146	0.2888	4.4877
0.7301	0.0087	9.7	0.0173	32.4910	0.5135	0.2618	4.2077
0.8315	0.0067	7.5	0.0126	24.8903	0.4163	0.1946	3.2736
0.9313	0.0038	3.7	0.0058	13.9802	0.3266	0.0844	1.5877
1.0000	0.0000	0.00	0.0000	0.0000	0.0000	0.0000	0.0000
isopropyl benzene + n-propyl benzene							
0.0000	0.0000	0.00	0.0000	0.0000	0.0000	0.0000	0.0000
0.1193	0.0015	0.6	0.0015	12.7856	0.3183	0.0667	0.9631
0.2209	0.0030	1.2	0.0032	21.7225	0.5700	0.1384	1.7335
0.3312	0.0044	1.7	0.0045	28.9243	0.8204	0.2041	2.3545
0.4397	0.0053	2.0	0.0053	33.2048	0.9713	0.2507	2.7297
0.5319	0.0058	2.0	0.0056	34.4569	1.1496	0.2720	2.8523
0.6395	0.0057	1.8	0.0054	32.9167	0.8108	0.2709	2.7525
0.7301	0.0051	1.5	0.0049	28.9318	0.5731	0.2444	2.4543
0.8315	0.0037	0.9	0.0038	21.3551	0.4211	0.1829	1.8752
0.9313	0.0015	0.1	0.0017	10.4797	0.3376	0.0851	1.0395
1.0000	0.0000	0.00	0.0000	0.0000	0.0000	0.0000	0.0000
isopropyl benzene + t-butyl benzene							
0.0000	0.0000	0.00	0.0000	0.0000	0.0	0.0000	0.0000
0.1193	0.0010	0.9	0.0012	14.1506	0.7048	0.0445	0.5832
0.2209	0.0023	1.5	0.0026	24.3469	1.1378	0.1614	0.9137
0.3312	0.0036	2.0	0.0038	32.6084	1.4736	0.3483	1.1795
0.4397	0.0045	2.3	0.0047	37.5872	1.6979	0.5453	1.3356
0.5319	0.0049	2.3	0.0052	39.1406	1.9101	0.6867	1.3780
0.6395	0.0049	2.1	0.0051	37.5850	1.6254	0.7796	1.3133
0.7301	0.0043	1.8	0.0045	33.2588	1.3577	0.7648	1.1562
0.8315	0.0031	1.2	0.0032	24.9198	1.0356	0.6107	0.8607
0.9313	0.0011	0.4	0.0011	12.8774	0..6028	0.2803	0.4383
1.0000	0.0000	0.00	0.0000	0.0000	0.0000	0.0000	0.0000
isopropyl benzene + biphenyl							
0.0000	0.0000	0.00	0.0000	0.0000	0.0000	0.0000	0.0000
0.1193	0.0028	1.0	0.0125	16.5386	3.6277	0.1241	0.5812
0.2209	0.0046	1.7	0.0245	28.5802	6.0471	0.2346	1.0269
0.3312	0.0060	2.2	0.0349	37.8051	7.8560	0.3094	1.3341
0.4397	0.0067	2.5	0.0419	42.8483	8.8932	0.3401	1.4698

Mole fraction 1,3-Dioxolane (x_1)	**Excess adiabatic compressibility $\beta_{ad}^E \times 10^{-7}$/ Pa^{-1}**	**Excess refractive index (n^E) × 10^4**	**Excess Free Volume $V_f^E \times 10^{-7}$ M^3mol^{-1}**	**Excessinternal pressure p_i^E × 10^5/ N m^{-2}**	**Excess Enthalpy H^E × 10^{-4} (J.mol^{-1})**	**Excess Surface tension (S^E) × 10^5 / N.m^{-1}**	**Excess Acoustic impedance (Z^E) × 10^{-2}g.cm.s^{-1}**
0.5319	0.0068	2.5	0.0448	43.8987	9.0729	0.3352	1.4649
0.6395	0.0063	2.3	0.0440	41.2588	8.2753	0.2960	1.3308
0.7301	0.0053	2.0	0.0394	35.7228	7.0948	0.2371	1.1194
0.8315	0.0037	1.4	0.0295	25.8405	5.0371	0.1456	0.7859
0.9313	0.0015	0.6	0.0142	12.2175	2.4339	0.0313	0.3676
1.0000	0.0000	0.00	0.0000	0.0000	0.0000	0.0000	0.0000

Utilizing these fundamental measurements, a series of critical derived thermodynamic and acoustic parameters were evaluated. The adiabatic compressibility (β_{ad}) was determined from the measured density and ultrasonic velocity using established acoustic relations [42, 43].

$$\beta_{ad} = u^{-2}\rho^{-1} \tag{4}$$

$$\beta_{ad}^E = \beta_{ad} - x_1\beta_{ad,1} - x_2\beta_{ad,2}, \tag{5}$$

The mixture, pure component 1, and pure component 2's isentropic compressibilities are denoted by $\beta_{ad.1}$ and $\beta_{ad.2}$ respectively.

The free volume (V_f) was evaluated based on the relationship between ultrasonic velocity and viscosity [44, 45].

$$V_f = (M\ U/\ k\ \eta)^{3/2} \tag{6}$$

Where M is the molecular weight (gm)

U is the sound velocity (cm/sec)

η is the viscosity (mPa.s)

k is the constant, equal to 4.28×10^9, independencetemperature as well as free volume V_f, the volume that is free isin milliliters per mole.

The internal pressure (p_i) was computed utilizing the standard free volume principle [46, 47].

$$p_i = bRT\left(\frac{k\eta}{u}\right)^{\frac{1}{2}} \frac{\rho^{\frac{2}{3}}}{M_{eff}^{\frac{7}{6}}} \tag{7}$$

Here, R is the universal gas constant, T is the absolute temperature, b is the packing factor (b = 2), and k is a constant that is independent of temperature and has a value of 4.28 × $10^9$for all liquids.

The following formula can be used to calculate the system's enthalpy (H):

$$H = V_m \times P_i \tag{8}$$

Acoustic impedance (Z) was obtained as the product of the medium's density and ultrasonic velocity [48],

$$Z = u \times \rho \tag{9}$$

While surface tension (S) was calculated using the Aurebach relation [49].

$$S = 6.4 \times 10^{-3}.\ \rho.u^{3/2} \tag{10}$$

Equation (10) was used to determine the surface tension of the system under study at 298.15 K using the measured density (ρ) and ultrasonic speed (u) of pure liquids and liquid mixtures.

The excess values for all these parameters were subsequently calculated by subtracting the ideal mixture values from the experimental mixture values.

$$A^E = A_{EXP.} - A_{IDEAL} \tag{11}$$

3.1. Excess Adiabatic Compressibility

The excess adiabatic compressibility (β_{ad}^E), serves as a highly sensitive indicator of the specific intermolecular interactions occurring within a mixed liquid system. The calculated (β_{ad}^E), values are detailed in Table 4, while Figure 2 graphically illustrates the variation of these values as a function of the cumene mole fraction (X_1).

Across the entire compositional range at 298.15 K, all six binary systems exhibit strictly positive deviations. As noted by Kiyohara and Benson [50], the behavior of (β_{ad}^E), is dictated by a complex balance of multiple opposing molecular effects. Generally, negative deviations arise from strong specific interactions that compact the liquid structure. Conversely, positive deviations indicate that mutual structure-breaking effects dominate the system.Similar outcomes in specific liquid mixtures others have also reported this., and these findings are in good accord with the present findings. The molecules' relative sizes, which permit more free volume in addition to fewer dipole-dipole interactions, could be the reason behind the positive observation values [51]. The consistently positive (β_{ad}^E), values observed here suggest that the mutual dispersion of the constituent molecules disrupts the inherent molecular associations present in the pure liquid states. According to Sri Devi et al. [52], the predominance of universal dispersion forces between dissimilar molecules is the primary driver for these positive values. Notably, the maximum positive deviation is observed in the cumene + mesitylene system. This pronounced effect can be attributed to significant steric hindrance; the presence of three methyl groups on the mesitylene ring prevents close molecular packing, thereby generating additional free volume and reducing dipole-dipole interactions. Ultimately, the positive (β_{ad}^E), values confirm that weak dispersive forces and geometric disparities heavily outweigh any specific associative interactions within these aromatic solvent systems.

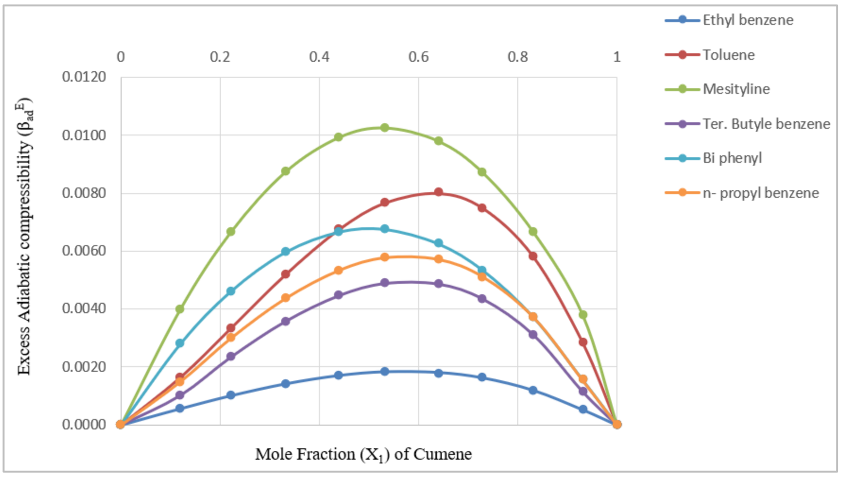

Figure 2. *Displays the excess adiabatic compressibility (β_{ad}^E) curves in relation to the mole fraction of isopropyl benzene (cumene, X_1) for binary combinations of isopropyl benzene (1) and aromatic hydrocarbons (2) at atmospheric pressure and 298.15 K. The values determined by applying the Redlich-Kister equation are symbolized by the solid lines.*

3.2. Excess Refractive Index

The excess refractive index (n^E) provides valuable insights into the compactness of molecular packing. As detailed in Table 4 and depicted in Figure 3, the n^E values are consistently positive across the entire composition range for all six binary systems at 298.15 K.

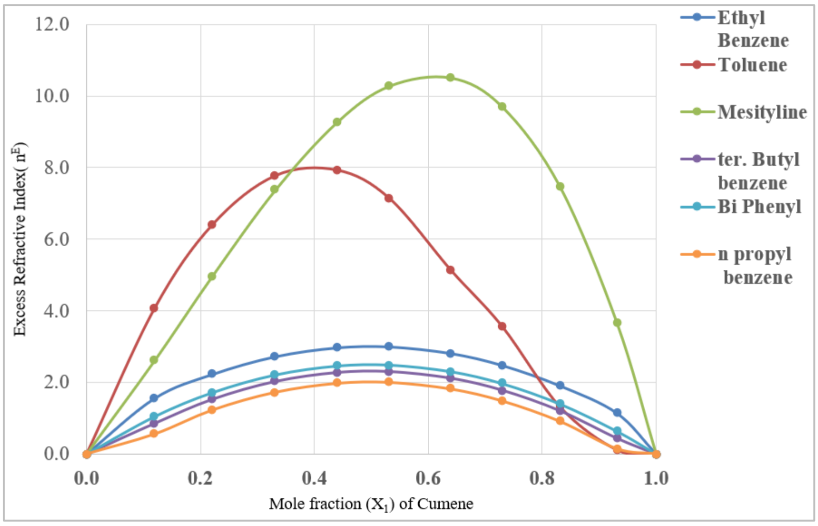

Figure 3. *Displays the excess refractive index (n^E) curves in relation to the mole fraction of isopropyl benzene (cumene, X_1) for binary combinations of isopropyl benzene (1) and aromatic hydrocarbons (2) at atmospheric pressure and 298.15 K. The values determined by applying the Redlich-Kister equation are symbolized by the solid lines.*

Generally, negative deviations in the refractive index are associated with specific interactions (such as hydrogen bonding or charge-transfer interactions) which lead to a decrease in free volume. Conversely, positive deviations are typically driven by non-specific dispersion forces. In the present study, the strictly positive (n^E) trends imply that the dispersive forces between the unlike molecules predominate. The disruption of the localized order of the pure liquids upon mixing leads to a less compact structural arrangement, which perfectly aligns with the positive deviations observed in the excess adiabatic compressibility.

3.3. Excess Free Volume

The excess free volume (V_f^E) serves as a macroscopic measure of the structural and spatial changes that occur during the mixing process. Table 4 and Figure 4 demonstrate that the calculated (V_f^E) values are entirely positive over the full mole fraction range for all evaluated systems at 298.15 K. Upon mixing, non-polar hydrocarbon molecules become dispersed within the cumene medium, leading to a reduction in dipole-dipole interactions among the methyl groups. The partial molar volume at infinite dilution reflects this effect, as reduced polar interactions almost always result in positive partial excess molar volumes. Since the majority of the examined mixtures show positive excess volumes, the experimental results support this theory. This implies that packing impacts brought on by geometrical constraints are subordinated to changes in intermolecular forces, which explains why different hydrocarbons have different excess volumes. Several patterns show up when comparing maximum excess volumes at equimolar composition: The highest excess free volume (V_f^E) is seen for cumene + mesitylene, where mesitylene has a flat geometry with three methyl groups in the meta positions around the aromatic ring; mixtures with non-flat or moderately substituted hydrocarbons (such as t-butyl benzene, isopropyl benzene) show intermediate values; and mixtures with flat or small-substituted hydrocarbons (such as ethyl benzene, mesitylene, and biphenyl). Steric and electronic effects can be used to qualitatively interpret these observations. The hydrocarbon molecules' bulky substituents weaken interactions and increase the excess volume by preventing the acetate groups from approaching closely. Toluene, ethyl benzene, mesitylene, and biphenyl, on the other hand, are flat molecules with few substituents that permit some residual interactions, leading to slightly positive, sigmoid, or even negative excess free volume (V_f^E). Three methyl groups in mesitylene create a steric hindrance that prevents cumene molecules from approaching, increasing the occupied volume and, consequently, the excess volume. Similar trends in excess volume with respect to molecular size and substitution have been observed for other non-polar + non-polar systems, such as mixtures of cumene with aromatic hydrocarbons.

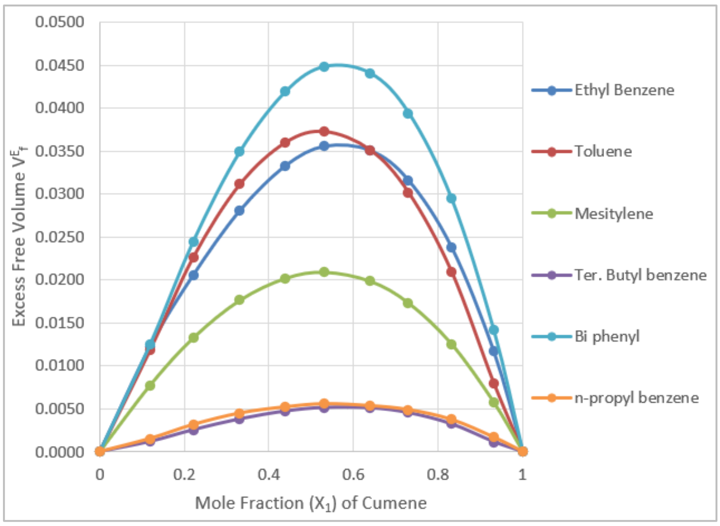

Figure 4. *Displays the excess free volume* (V_f^E) *curves in relation to the mole fraction of isopropyl benzene (cumene,* X_1*) for binary combinations of isopropyl benzene (1) and aromatic hydrocarbons (2) at atmospheric pressure and 298.15 K. The values determined by applying the Redlich-Kister equation are symbolized by the solid lines.*

The overall sign and magnitude of (V_f^E) are determined by the interplay of physical, chemical, and geometrical factors. Because isopropyl benzene (cumene) is weakly polar and the selected aromatic hydrocarbons are predominantly non-polar, the addition of the hydrocarbons effectively disperses the cumene molecules. This process weakens the localized dipolar interactions and disrupts the dispersive π-π interactions between the aromatic rings, a behavior that is consistent with observations in similar hydrocarbon mixtures [53, 54]. This disruption ultimately causes the overall volume of the mixture to expand. Comparing the mixtures at equimolar compositions reveals that the cumene + mesitylene system exhibits the highest(V_f^E). This occurs because the three symmetrically positioned methyl groups on the mesitylene ring create significant steric bulk, which physically prevents the cumene molecules from approaching closely and packing efficiently.

3.4. Excess Enthalpy

Excess enthalpy (H^E) is a crucial metric for evaluating the thermal effects of intermolecular interactions during the mixing process. The calculated H^E values for the binary systems are presented in Table 4, while Figure 5 illustrates the variation of H^E as a function of the cumene mole fraction (X_1) at 298.15 K.

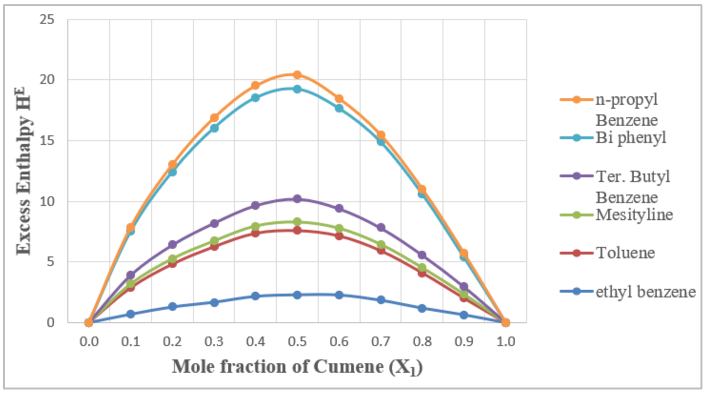

Figure 5. *Displays the excess enthalpy (H^E) curves in relation to the mole fraction of isopropyl benzene (cumene, X_1) for binary combinations of isopropyl benzene (1) and aromatic hydrocarbons (2) at atmospheric pressure and 298.15 K. The values determined by applying the Redlich-Kister equation are symbolized by the solid lines.*

Across all six binary mixtures, the excess enthalpy values are entirely positive and exhibit a parabolic trend, reaching a maximum at approximately an equimolar concentration. As outlined by Nakayama and Shinoda [55], the overall behavior of excess enthalpy reflects a complex balance between exothermic and endothermic processes. Negative contributions typically arise from the efficient geometrical fitting of molecules or the formation of new intermolecular dipolar interactions. Conversely, positive contributions result from endothermic processes, such as the rupture of hydrogen bonds or the disruption of dispersive interactions between the pure components. Because the selected aromatic hydrocarbons are nearly non-polar and cumene is only weakly polar, the strictly positive (H^E) values indicate that the energy required to break the existing dispersive π-π interactions between the pure aromatic rings is significantly greater than the energy released upon mixing [56]. Consequently, the mixing process is endothermic, confirming that the newly formed solute-solvent interactions are weaker than the cohesive forces present in the unmixed liquids.

3.5. Excess Internal Pressure

Internal pressure (p_i) serves as a macroscopic measure of the cohesive forces within a liquid, reflecting the equilibrium between attractive forces (such as hydrogen bonding, dipole-dipole, and dispersion interactions) and short-range repulsive forces. The calculated excess internal pressure (p_i^E). values are detailed in Table 4, and their concentration dependence is plotted in Figure 6. For all mixtures, the excess internal pressure$(p_i^E)$is positive over the entire composition range, indicating the predominance of weak intermolecular interactions. As the concentration of cumene increases in each system, the absolute magnitude of (p_i^E)decreases.

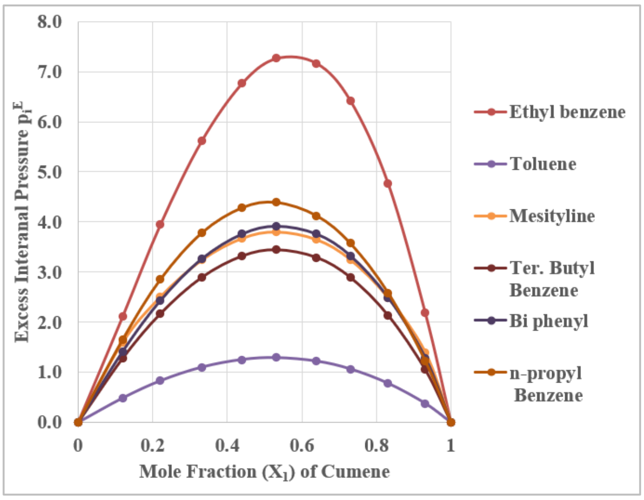

Figure 6. *Displays the excess internal pressures(p_i^E)curves in relation the mole fraction of isopropyl benzene (cumene, X_1) for binary combinations of isopropyl benzene (1) and aromatic hydrocarbons (2) at standard atmospheric pressure and 298.15 K. The values determined by applying the Redlich-Kister equation is a mathematical expression symbolized by the solid lines.*

For all evaluated binary systems, the (p_i^E).values are consistently positive across the entire composition range, which signifies a general weakening of cohesive forces upon mixing. The magnitude of these positive deviations follows the sequence: ethyl benzene > toluene > mesitylene > n-propyl benzene > tert-butyl benzene > biphenyl. This trend suggests that the cumene + ethyl benzene system experiences the most significant disruption of internal pressure, whereas the cumene + biphenyl system is the least affected. In mixtures of cumene and aromatic hydrocarbons, the predominant specific interactions are likely of the electron donor-acceptor (charge-transfer) variety, where the π-electrons of the cumene ring function as donors and the π-electrons of the secondary aromatic rings act as acceptors [57]. Notably, as the number of electron-donating methyl substituents on the aromatic ring increases (e.g., moving from benzene to mesitylene), the magnitude of(p_i^E).decreases. Methyl groups release electron density into the aromatic ring, which diminishes the ring's capacity to accept electrons from cumene. This behavior is explained by the methyl groups' ability to release electrons, which increases the aromatic ring's electron density while concurrently declining its capacity to accept electrons. Lower $(p_{\mathrm{i}}^{\mathrm{E}})$ values result from the donor-acceptor weakening of connections between dissimilar molecules as the quantity of methyl groups increases. Binary combinations of aromatic hydrocarbons and tetra hydro furan have demonstrated comparable patterns in excess free volume $(V_f^E)$and excess internal pressure$(p_{\mathrm{i}}^{\mathrm{E}})$. The compositional trends this knowledge of molecular interactions, as seen in the excess internal pressure$(p_{\mathrm{i}}^{\mathrm{E}})$, offers a satisfactory explanation of values for the current systems. This dampens the charge-transfer interactions between the dissimilar molecules, a phenomenon that mirrors previously reported trends for mixtures of tetra hydro furan and aromatic hydrocarbons [58].

3.6. Excess Acoustic Impedance

Table 3 shows the corresponding acoustic impedance (Z) values. The proportion of each particle's immediate excess pressures in the medium to the particle's immediate velocity is referred to as the medium's acoustic impedance (Z). Pressure varies from particle to particle as a sound wave travels through a material. The elastic and inertial properties of the medium govern this component. Table 3 demonstrates that the observed decrease in acoustic impedance with increasing isopropyl benzene (cumene) concentration in each of the six binary liquid systemsindicates a decline inthe structural compactness of the medium, a rise in free volume, as well asthe dominance of weak-solvent interactions. The acoustic impedance points' apparent decrease either more free volume or weaker particular contacts. Acoustic impedance (Z) evaluates the specific resistance of a medium to the propagation of sound waves and is heavily governed by the inertial and elastic properties of the fluid [59]. Because this parameter is directly tied to the molecular packing and structural compactness of the system [60], the excess acoustic impedance (Z^E) serves as a valuable diagnostic tool for assessing intermolecular interactions.

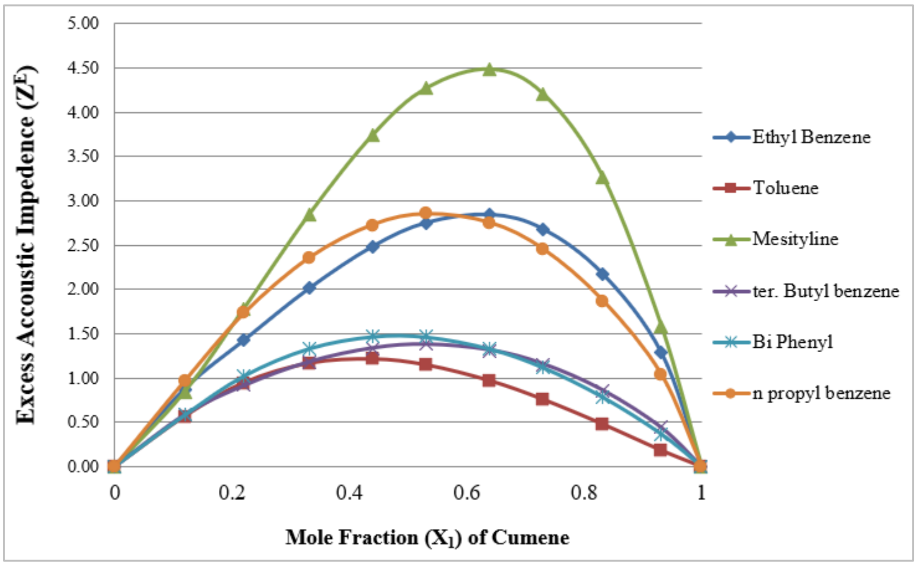

Figure 7. *Displays the excess acoustic impedance* (Z^E) *curves in relation to the mole fraction of isopropyl benzene (cumene,* X_1*) for binary combinations of isopropyl benzene (1) and aromatic hydrocarbons (2) at atmospheric pressure and 298.15 K. The values determined by applying the Redlich-Kister equation are symbolized by the solid lines.*

As illustrated in Figure 7 and detailed in Table 4, the calculated (Z^E) values are distinctly positive for all six binary mixtures at 298.15 K. In thermodynamic studies, positive deviations in acoustic impedance are typically indicative of structure-breaking effects and relatively weak intermolecular forces [61]. The introduction of the aromatic hydrocarbons disrupts the localized arrangement of the cumene molecules. The resulting interactions between the dissimilar species—primarily weak dipole-induced dipole and weak π-π interactions—are insufficient to re-establish a highly ordered molecular structure [62-64]. Consequently, the overall structural compactness of the medium decreases, corroborating the positive deviations observed in both the free volume and adiabatic compressibility.

3.7. Excess Surface Tension

Surface tension (S) is a fundamental physicochemical property that heavily influences macroscopic processes such as mass transfer and heat exchange [65]. The excess surface tension (S^E) for the evaluated systems was calculated using standard empirical relations, with the resulting data presented in Table 4 and plotted in Figure 8. Table 3 presents the calculated surface tension (S) values for pure isopropyl benzene (cumene), ethyl benzene, toluene, mesitylene, *n*-propyl benzene, *tert*-butyl benzene, and biphenyl, along with their corresponding binary mixtures. Across the entire composition range, the surface tension (S) decreases nearly linearly with increasing mole fraction of isopropyl benzene (cumene) (Table 3). Table 4 summarizes the excess surface tension data, while Figure 8 has been constructed using the calculated surface tension (S) values. Figure 8 illustrates that, with an increase in mole fraction (x_1), the surface tension (S) increases, which may be attributed to the higher proportion of isopropyl benzene (cumene) in the mixture. This behavior is likely associated with enhanced π-π interactions, leading to an increase in surface tension. The surface tension values of isopropyl benzene (cumene) were calculated using Eq. (10) [49], and the results are presented in Table 3. Furthermore, the analysis based on excess surface tension (S^E). Furthermore, the excess surface tension (S^E) is positive over the entire composition range. This positive deviation indicates that the more surface-active components preferentially remain in the bulk phase rather than accumulating at the interface. Such behavior arises due to changes in intermolecular interactions either repulsive or weakly attractive between unlike molecules, leading to positive surface tension deviations.

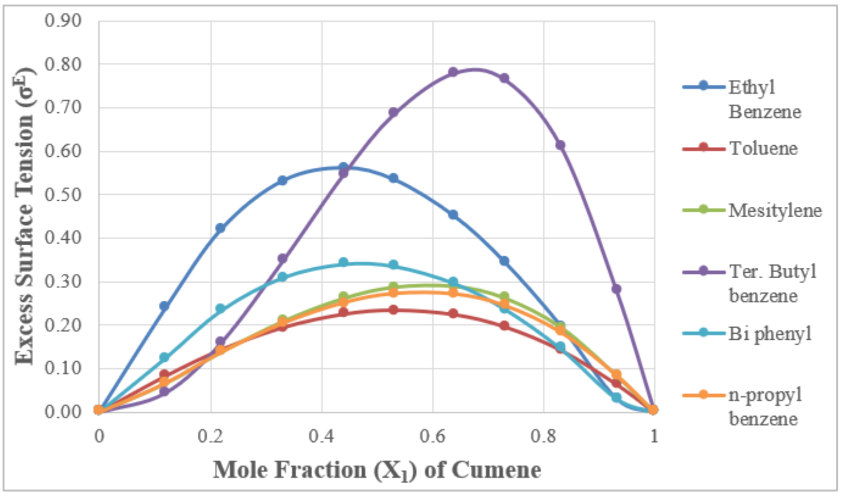

Figure 8. *Displays the excess surface tension (S^E)curves in relation to the mole fraction of isopropyl benzene (cumene, X_1) for binary combinations of isopropyl benzene (1) and aromatic hydrocarbons (2) at atmospheric pressure and 298.15 K. The values determined by applying the Redlich-Kister equation are symbolized by the solid lines.*

Across the entire mole fraction range at 298.15 K, the (S^E) values are strictly positive for all six binary mixtures. Positive deviations in surface tension typically occur when the active components migrate toward the surface region due to changes in the attractive or repulsive forces between the dissimilar molecules in the bulk fluid. Interestingly, the surface behavior of these specific aromatic systems appears to be heavily dictated by their volumetric and compressibility characteristics rather than solely by direct solute-solvent interactions at the interface [66, 67]. The positive S^E trends indicate that the cohesive forces at the liquid-air interface are stronger than the disrupted intermolecular forces within the bulk mixture.

In the whole spectrum of mole fractions, the values of (V_f^E),(p_i^E),(H^E),(n^E),(S^E), (Z^E) and$(\beta_{ad}^E)$are positive for mixtures of isopropyl benzene (cumene) + ethyl benzene, isopropyl benzene (cumene) + toluene, isopropyl benzene (cumene) + mesitylene, isopropyl benzene (cumene) + n-propyl benzene, isopropyl benzene (cumene) + tert-butyl benzene, and isopropyl benzene (cumene) + biphenyl.

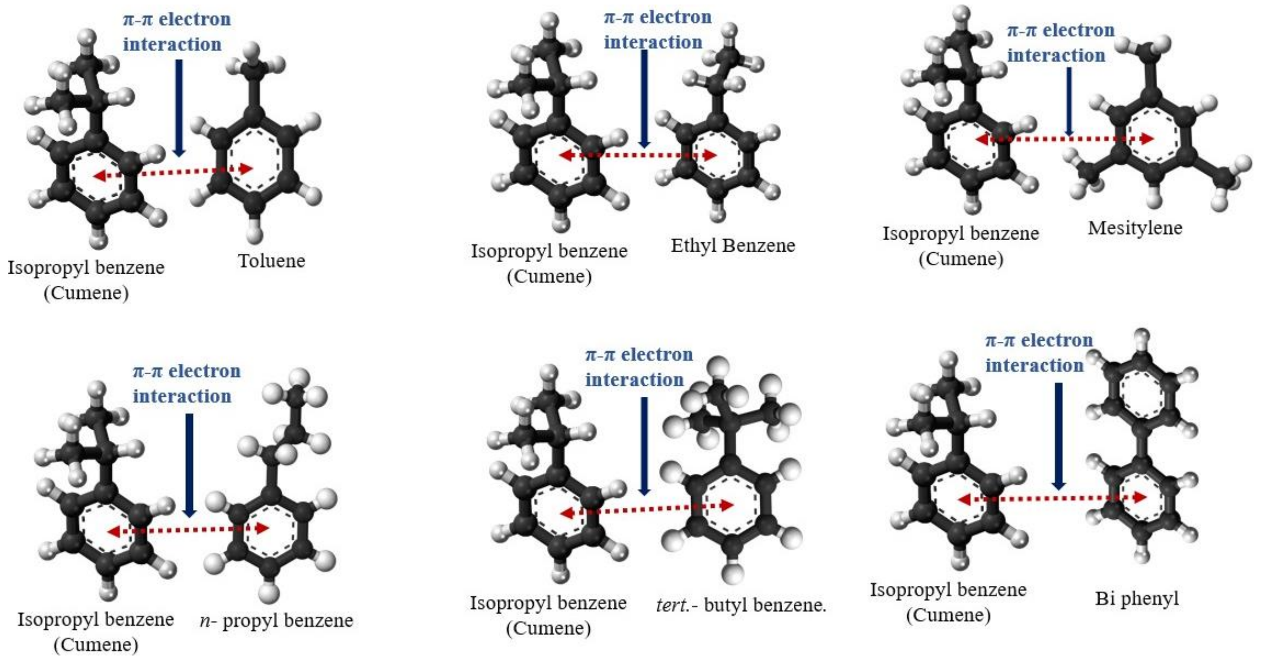

Figure 9. *The schematic structural presentation of the interactions between isopropyl benzene (cumene) and aromatic hydrocarbon molecules.*

4. Conclusion

This comprehensive study successfully investigated the concentration-dependent thermo physical and acoustic behaviors of six binary liquid systems, comprising isopropyl benzene (cumene) paired with ethylbenzene, toluene, mesitylene, n-propyl benzene, tert-butyl benzene, and biphenyl. By systematically measuring fundamental baseline properties—specifically density, viscosity, ultrasonic velocity, and refractive index—at a constant temperature of 298.15 K and atmospheric pressure, a robust dataset was generated. These empirical metrics enabled the precise evaluation of critical derived thermodynamic parameters, including adiabatic compressibility, free volume, internal pressure, enthalpy, acoustic impedance, and surface tension. The subsequent calculation of excess thermodynamic functions revealed strictly positive deviations across the entire compositional range for all six binary mixtures. This uniform trend provides compelling macroscopic evidence of a predominant structure-breaking effect upon mixing. The introduction of the selected aromatic hydrocarbons effectively disperses the weakly polar cumene molecules, disrupting their localized dipolar ordering and breaking the cohesive π-π dispersive interactions present in the pure liquid states. Furthermore, the energetic and cohesive metrics specifically the positive excess enthalpy (H^E) and positive excess internal pressure),$\left(p_i^E\right)$, confirm that the mixing process is endothermic. The energy required to dismantle the specific self-associated structures of the unmixed liquids significantly outweighs the energy released by the formation of new, relatively weak dipole-induced dipole and charge-transfer interactions between the dissimilar molecules. The positive deviations in excess acoustic impedance (Z^E) and adiabatic compressibility (β_{ad}^E) further corroborate this, indicating a notable decrease in the structural compactness and acoustic rigidity of the fluid mediums.

A key highlight of this research is the pronounced influence of molecular geometry and steric hindrance on the interaction dynamics. As the bulkiness or the alkyl chain length of the substituted aromatic hydrocarbon increases, the molecules are physically prevented from achieving close, efficient packing. This steric effect is most vividly demonstrated by the mesitylene system, where the symmetrical methyl groups generate significant free volume and actively hinder electron donor-acceptor interactions. Consequently, based on the magnitude of the derived excess properties, the overall strength of intermolecular interactions in these systems strictly follows the sequence: ethylbenzene> toluene >mesitylene> n-propyl benzene > tert-butyl benzene> biphenyl. Ultimately, these findings establish a rigorous quantitative foundation for understanding non-ideal behavior and localized molecular clustering within complex aromatic mixtures. As aromatic liquids are increasingly utilized in advanced solvent design, energy storage, and chemical synthesis, the thermo physical data reported herein hold significant practical value. Future research expanding upon this work—through the investigation of ternary mixtures, the application of complementary spectroscopic techniques, and the execution of computational molecular modeling across wider temperature ranges—will further validate these thermodynamic frameworks and enhance industrial separation protocols.

Abbreviation

ρ	Density of the mixture ($g.cm^{-3}$)
u	Sound speed of the mixture ($m.s^{-1}$)
u^E	Excess Sound Velocity ($m.s^{-1}$)

η	Viscosity (m.Pas)
M	Molar mass
T	Temperature
P	Pressure
V	Volume
η^E	Excess Viscosity (m.Pas)
T	Temperature (Kelvin)
n	Refractive index of the mixture
n^E	Excess refractive index
(β_{ad})	Adiabatic compressibility (Pa^{-1})
(β_{ad}^E)	Excess adiabatic compressibility(Pa^{-1})
(H)	Enthalpy ($J.mol^{-1}$)
(H^E)	Excess enthalpy ($J.mol^{-1}$)
(V_f)	Free volume ($M^3 mol^{-1}$)
(V_f^E)	Excess free volume, ($M^3 mol^{-1}$)
(P_i)	Internal pressure ($N\ m^{-2}$)
(p_i^E)	Excess internal pressure ($N\ m^{-2}$)
(S)	Surface tension ($N.m^{-1}$)
(S^E)	Excess surface tension ($N.m^{-1}$)
(Z)	Acoustic impedance ($g.cm.s^{-1}$)
(Z^E)	Excess acoustic impedance ($g.cm.s^{-1}$)
Y^E	Thermodynamic excess function
X_1	Mole Fraction of isopropyl benzene (Cumene)

Acknowledgments

The authors gratefully acknowledge to Uttar Pradesh Council of Science and Technology, Lucknow (No. CST/CHEM/D-648 dated 01/08/2024) for financial support (Project ID: 3409).

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Chandrapal Prajapati: Conceptualization, Formal analysis, Investigation, Supervision, Validation, Visualization,

Suneel Kumar: Conceptualization, Formal analysis, Resources, Software

Data Availability Statement

The data that has been used is confidential.

Conflicts of Interest

The authors declare no conflicts of interest.

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